ESD-TR-67-336

Technical Note 1967-39

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Finite Temperature Theory for the Attenuation of Quasi-Particle Excitations in Real Metals

14 August 1967

Prepared under Electronic Systems Division Contract AF 19(628)-5167 by

Lincoln Laboratory

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Lexington, Massachusetts

The work reported in this document was performed at Lincoln Laboratory, a center for research operated by Massachusetts Institute of Technology, with the support of the U.S. Air Force under Contract AF 19(628)-5167.

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ABSTRACT

The finite temperature generalization of the Quinn, Adler theory for the decay rate of electronic excitations in a normal Fermion system is presented. The theory is developed in terms of quasi-particle parameters and without restriction to a particular approximation, such as RPA, for the dielectric response of the system. The relations derived are pertinent to the lifetime problem in real solids; in particular, local field effects are rigorously taken into account.

Accepted for the Air Force
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Finite Temperature Theory for the Attenuation of Quasi-Particle Excitations in Real Metals

INTRODUCTION

Several years ago Adler[1] presented a theory for the attenuation rate of hot electrons in metals. The theory was developed along lines similar to the earlier work of Quinn and Ferrell,[2] and Quinn[3] concerning the properties of an interacting electron gas. All of the above calculations were carried out for the case of zero temperature. As far as we know, the corresponding extension of the theory to finite temperature has not been given in a general context. It is the purpose of this note to simply provide such a generalization, in a form relevant for band electrons in solids. Let us comment at once that, for the case of truly hot electrons, finite temperature corrections cannot be very important. It is only for the case of low-lying excitations that these effects need be taken into account. Furthermore, because we are concerned only with low energy excitations, we may consistently formulate the theory in terms of quasi-particle energies.

For the most part, the results presented in this note are formal. For the case of free electrons at sufficiently low temperature, it is known[4] that the decay rate for low-lying quasi-particle excitations must have exactly the form

$$\Gamma_{\vec{k}}(\epsilon) = C_{\vec{k}}[(\epsilon-\mu)^2 + \pi^2(k_B T)^2] \ .$$

A brief discussion of this result, within the framework of a simple RPA treatment is presented in Appendix A. Qualitatively, one expects to find a similar result for the case of normal simple metals. In particular, the

results for low energy excitations obtained by Adler, barring the more pathological cases, e.g., a cylindrical Fermi surface, which he has discussed, may, with suitable assumptions, be shown to generalize at finite temperature in a manner analogous to that presented in Appendix A.

Finally, in real solids, one expects the damping due to electron-phonon interaction to be comparable in magnitude to the effects we are considering here. This problem may, however, be handled in a parallel manner. A rather thorough discussion of the electron-phonon interaction at finite temperature, based on a model of free electrons interacting with longitudinal acoustic phonons, may be found in the book by Abrikosov, et al.[5]

GENERAL THEORY

Our theoretical approach is based on the well-known finite temperature perturbation theory as developed by Luttinger and Ward,[6] and Luttinger.[7,8] In this section we give a brief review of the relevant propagator formalism.

We take the Hamiltonian to be of the standard form

$$H = H_o + H' \quad , \tag{1}$$

with

$$H_o = \sum_r \epsilon_r a_r^\dagger a_r \quad , \tag{2}$$

$$H' = \frac{1}{2} \sum_{rss'r'} (rs|v|r's') a_r^\dagger a_s^\dagger a_{s'} a_{r'}$$

$$= \frac{1}{2V} \sum_{\vec{q}} v(\vec{q}) \sum_{rsr's'} \rho(\vec{q})_{rr'} \rho(-\vec{q})_{ss'} a_r^\dagger a_s^\dagger a_{s'} a_{r'} \quad , \tag{3}$$

where $v(\vec{q}) = 4\pi e^2/q^2$ and $\rho(\vec{q})_{rr'} = \langle r | e^{i\vec{q}\cdot\vec{x}} | r' \rangle$.

Next we define the exact single particle propagator and polarization propagator[9,10] respectively as

$$g'_{rr'}(\beta',\beta'') = \mathrm{Tr}\{e^{-\beta(H-\mu N-\Omega)} T[a^{\dagger}_{r'}(\beta')_H \, a_r(\beta'')_H]\} \quad , \tag{4}$$

$$P_{\vec{q}\vec{q}'}(\beta',\beta'') = \frac{1}{V} \mathrm{Tr}\{e^{-\beta(H-\mu N-\Omega)} T[\rho_{\vec{q}'}(\beta')_H \, \rho_{-\vec{q}}(\beta'')_H]\} \quad , \tag{5}$$

where $\beta \geq \beta'$, $\beta'' \geq 0$ and all operators are in the Heisenberg representation, e.g.,

$$\rho_{\vec{q}'}(\beta')_H = e^{\beta' H} \rho_{\vec{q}'} e^{-\beta' H}$$

$$= \sum_{rr'} \rho(\vec{q}')_{rr'} \, a^{\dagger}_r(\beta')_H \, a_{r'}(\beta')_H \quad . \tag{6}$$

Making use of the cyclic invariance of the trace in these expressions, one obtains the Fourier representations

$$g'_{rr'}(\beta',\beta'') = \frac{1}{\beta} \sum_{\ell} S'_{rr'}(z_\ell) \, e^{z_\ell(\beta'-\beta'')} \quad , \tag{7}$$

$$P_{\vec{q}\vec{q}'}(\beta',\beta'') = \frac{1}{\beta} \sum_{\ell} \Pi'(\xi_\ell)_{\vec{q}\vec{q}'} \, e^{\xi_\ell(\beta'-\beta'')} \quad , \tag{8}$$

where $z_\ell = \pi i(2\ell+1)/\beta + \mu$, $\xi_\ell = 2\pi i\ell/\beta$ and ℓ takes on all integer values.

In perturbation theory, $S'_{rr'}(z_\ell)$ is given by the sum of all electron propagator diagrams in which a Fermion line labeled r' enters and a line labeled r emerges. Likewise, $\Pi'(\xi_\ell)_{\vec{q}\vec{q}'}$ is given by the sum of all

polarization diagrams in which an interaction line labeled $\vec{q}\,'$ enters and a line labeled $\vec{q}$ emerges (the external lines not being part of Π'). Furthermore, S and Π' satisfy their respective Dyson equations

$$S'_{rr'}(z_\ell) = S_r(z_\ell)\delta_{rr'} + S_r(z_\ell)\sum_{r_1} G_{rr_1}(z_\ell)S'_{r_1r'}(z_\ell) \quad , \tag{9}$$

$$\Pi'(\xi_\ell)_{\vec{q}\vec{q}\,'} = \Pi(\xi_\ell)_{\vec{q}\vec{q}\,'} - \sum_{\vec{q}_1} \Pi(\xi_\ell)_{\vec{q}\vec{q}_1} v(\vec{q}_1)\Pi'(\xi_\ell)_{\vec{q}_1\vec{q}\,'} \quad , \tag{10}$$

where G is the proper self-energy function and Π is the proper polarization function. Now we may label the states $|r\rangle$ as $|\vec{k}\gamma\sigma\rangle$ where σ is a spin index, γ is a band index, and where the wavevector $\vec{k}$ is confined to the first zone. In this reduced zone scheme, S' and G will be diagonal in the wavevector index, but will have off-diagonal elements in the band indices. Likewise, from quite general symmetry considerations, Π' and Π have off-diagonal elements only for $\vec{q}$'s differing by a reciprocal lattice vector.

Finally, we may write down the very useful spectral representations of the propagators $S'_{rr'}(z_\ell)$ and $\Pi'(\xi_\ell)_{\vec{q}\vec{q}\,'}$, which are

$$S'_{rr'}(z_\ell) = \int_{-\infty}^{\infty} dE \, \frac{A(E)_{rr'}}{z_\ell - E} \quad , \tag{11}$$

$$\Pi'(\xi_\ell)_{\vec{q}\vec{q}\,'} = \int_{-\infty}^{\infty} dE \, \frac{B(E)_{\vec{q}\vec{q}\,'}}{E - \xi_\ell} \quad . \tag{12}$$

These relations are obtained in the usual manner by evaluating (4) and (5) in the representation $|n\rangle$ of exact eigenstates of H, and then inverting (7) and (8) to obtain the corresponding Fourier coefficients. The spectral

density functions $A(E)_{rr'}$ and $B(E)_{\vec{q}\vec{q}'}$ are given in Appendix B, along with their various general sum rules. One important property of the spectral density functions is

$$A(E)_{rr'}^{*} = A(E)_{r'r} \quad , \tag{13}$$

$$B(E)_{\vec{q}\vec{q}'}^{*} = B(E)_{\vec{q}'\vec{q}} \quad , \tag{14}$$

i.e., the diagonal elements are real.

ELECTRON SELF-ENERGY

We now proceed to calculate the electron self-energy in the approximation which retains only the lowest order vertex function. In this approximation, one obtains, using the well-known graphical rules,

$$G_{rr'}(z_\ell) = G^{(1)}_{rr'} + G^{(2)}_{rr'}(z_\ell) \quad , \tag{15}$$

where $G^{(1)}_{rr'}$ is a constant, independent of z_ℓ, and is given by

$$G^{(1)}_{rr'} = \sum_{ss'} [(rs|v|r's') - (rs|v|s'r')] \cdot \frac{1}{\beta} \sum_{\ell'} S_{s's}(z_{\ell'}) e^{z_{\ell'} 0+} \quad . \tag{16}$$

This term is clearly a generalization of the usual Hartree-Fock self-energy, and is intimately connected with one of the sum rules satisfied by the electron spectral density function (see Appendix B). The second term in Eq. (15) is more interesting. This term is usually associated

with electron correlation, and is given by

$$G^{(2)}_{rr'}(z_\ell) = \frac{1}{V}\sum_{\vec{q}\vec{q}'} v(\vec{q})\,v(\vec{q}\,')\sum_{ss'} \rho_{rs'}(\vec{q})\,\rho_{sr'}(-\vec{q}\,')$$

$$\frac{1}{\beta}\sum_{\ell'} S'_{s's}(z_\ell - \xi_{\ell'})\,\Pi'(\xi_{\ell'})_{\vec{q}\vec{q}'} \quad . \tag{17}$$

Now, as Luttinger has discussed, we should seek a similarity transformation which diagonalizes the matrix $\varepsilon_r \delta_{rr'} + G_{rr'}(z_\ell)$. This is almost surely unfeasible to obtain in practice, and perhaps even in principle, i.e., it is not known whether such a transformation even exists in general. Therefore, in order to obtain something tractable, we shall proceed by simply assuming that the off-diagonal elements of G (and hence also of S′) may be neglected.

Because $G^{(1)}_r$ is real, this term does not contribute directly to the electronic attenuation rate, i.e., its effect is simply to modify the quasi-particle dispersion spectrum. Turning to the consideration of $G^{(2)}_r(z_\ell)$, we may invoke the spectral representations of the propagators S′ and Π′ and obtain

$$G^{(2)}_r(z_\ell) = \frac{1}{V}\sum_{\vec{q}\vec{q}'} v(\vec{q})\,v(\vec{q}\,')\sum_{s} \rho_{rs}(\vec{q})\,\rho_{sr}(-\vec{q}\,')$$

$$\cdot \int_{-\infty}^{\infty} dE\, dE'\, B(E')_{\vec{q}\vec{q}'}\, A(E)_s\, \frac{1}{\beta}\sum_{\ell'} \frac{1}{\xi_{\ell'} - E'}\;\frac{1}{\xi_{\ell'} - z_\ell + E} \quad . \tag{18}$$

The $\xi_{\ell'}$ sum in this expression is now trivially done using the standard prescription

$$\frac{1}{\beta}\sum_{\ell} F(\xi_\ell) = -\left\{ \begin{array}{c} \text{sum of residues of} \\ F(\xi)N(\xi) \text{ at poles of } F(\xi) \end{array} \right\} , \qquad (19)$$

where $N(\xi) = (e^{\beta\xi}-1)^{-1}$ is the Bose function, and $F(\xi)$ has only simple poles. Using this prescription, we have

$$\frac{1}{\beta}\sum_{\ell'} \frac{1}{\xi_{\ell'}-E'} \; \frac{1}{\xi_{\ell'}-z_\ell+E}$$
$$= \frac{f^+(E)\,N'(E') + f^-(E)\,N(E')}{z_\ell - E - E'} , \qquad (20)$$

with $N'(E') = N(E') + 1$. Having carried out the $\xi_{\ell'}$ sum we may now continue $G_r^{(2)}(z_\ell)$ off the set of points z_ℓ. The (unique) continuation which has no essential singularity at infinity may then be written

$$G_r^{(2)}(z) = \frac{1}{V}\sum_{\vec{q}\vec{q}'} v(\vec{q})\,v(\vec{q}')\sum_s \rho_{rs}(\vec{q})\,\rho_{sr}(-\vec{q}')$$

$$\int_{-\infty}^{\infty} dE\,dE'\,B(E')_{\vec{q}\vec{q}'}\,A(E)_s \; \frac{f^+(E)N'(E')+f^-(E)N(E')}{z - E - E'} . \qquad (21)$$

We note that the function defined by (21) is analytic except on the real z-axis. Furthermore, from (13) and (14), we see $G_r^{(2)}(z)^* = G_r^{(2)}(z^*)$, i.e., there is a pure imaginary discontinuity across the real z-axis. Thus, for z near the real axis, we have

$$G_r^{(2)}(\varepsilon \mp is)$$

$$= \frac{1}{V} \sum_{\vec{q}\,\vec{q}\,'} v(\vec{q})\, v(\vec{q}\,') \sum_s \rho_{rs}(\vec{q})\, \rho_{sr}(-\vec{q}\,')$$

$$\cdot \int_{-\infty}^{\infty} dE\, dE'\, B(E')_{\vec{q}\,\vec{q}\,'}\, A(E)_s\, \frac{f^+(E)\, N'(E') + f^-(E)\, N(E')}{\varepsilon - E - E' \mp is}\ , \tag{22}$$

and hence

$$\operatorname{Im} G_r^{(2)}(\varepsilon \mp is)$$

$$= \pm \frac{\pi}{V} \sum_{\vec{q}\,\vec{q}\,'} v(\vec{q})\, v(\vec{q}\,') \sum_s \rho_{rs}(\vec{q})\, \rho_{sr}(-\vec{q}\,')$$

$$\int_{-\infty}^{\infty} dE\, B(\varepsilon - E)_{\vec{q}\,\vec{q}\,'}\, A(E)_s \tag{23}$$

$$[f^+(E)\, N'(\varepsilon - E) + f^-(E)\, N(\varepsilon - E)]$$

From the spectral representation of $\Pi'(\xi_\ell)_{\vec{q}\,\vec{q}\,'}$, it is then easy to see that this result may be written

$$\operatorname{Im} G_r^{(2)}(\varepsilon \mp is)$$

$$= \mp \operatorname{Im} \frac{1}{V} \sum_{\vec{q}\,\vec{q}\,'} v(\vec{q})\, v(\vec{q}\,') \sum_s \rho_{rs}(\vec{q})\, \rho_{sr}(-\vec{q}\,')$$

$$\int_{-\infty}^{\infty} dE\, \Pi'(\varepsilon - E - is)_{\vec{q}\,\vec{q}\,'}\, A(E)_s\, [f^+(E)\, N'(\varepsilon - E) + f^-(E)\, N(\varepsilon - E)]\ . \tag{24}$$

The functions $G_r(\varepsilon \mp is)$ correspond to the well-known advanced and retarded self-energy.

Now for ϵ near μ, the statistical factors in (24) constrain E to values near μ, and for such values, we assume that $A(E)_s = \frac{1}{\pi} \operatorname{Im} S_s'(E-is)$ is a sharply peaked function, i.e., we assume

$$
\begin{aligned}
A(E)_s &\simeq \delta[E-\epsilon_s-\Delta_s(E)] \\
&\simeq Z_s\,\delta(E-E_s) \quad ,
\end{aligned}
\tag{25}
$$

where Δ is the real part of the self-energy, $Z_s = \left[1 - \frac{\partial \Delta_s(E)}{\partial E}\right]^{-1}_{E_s}$,
and E_s is the (we assume unique) quasi-particle energy given by the solution of

$$
E_s - \epsilon_s - \Delta_s(E_s) = 0 \quad . \tag{26}
$$

As always, the ultimate justification of Equation (25) must be the self-consistency of the final result.

Using this approximation, we obtain for the imaginary part of G

$$
\operatorname{Im} G_r(\epsilon \mp is) = \mp \operatorname{Im} \frac{1}{V} \sum_{\vec{q}\vec{q}\,'} v(\vec{q}\,') \sum_s Z_s\, \rho_{rs}(\vec{q})\rho_{sr}(-\vec{q}\,')
$$

$$
\cdot\, \Pi'(\epsilon-E_s-is)_{\vec{q}\vec{q}\,'}\, [f^+(E_s)N'(\epsilon-E_s) + f^-(E_s)N(\epsilon-E_s)] \quad . \tag{27}
$$

Now $\operatorname{Im} G_r(\epsilon+is)$ and $\operatorname{Im} G_r(\epsilon-is)$ are related to the damping rate for particle and hole propagation respectively. In either case, because these functions differ only in sign, we shall simply assess the lifetime for the corresponding excitation through the relation

$$\tau_r^{-1} = \frac{2Z_r}{\hbar}\,\Gamma_r(E_r) \quad , \tag{28}$$

with

$$\begin{aligned}\Gamma_r(E_r) &= \mathrm{Im}\,G_r(E_r - is)\\ &= -\,\mathrm{Im}\,\frac{1}{V}\sum_{\vec{q}\vec{q}'} v(\vec{q})\,v(\vec{q}')\sum_s Z_s\,\rho_{rs}(\vec{q})\,\rho_{sr}(-\vec{q}')\\ &\quad\cdot\,\Pi'(E_r - E_s - is)_{\vec{q}\vec{q}'}\,[f^+(E_s)N'(E_r - E_s) + f^-(E_s)N(E_r - E_s)] \quad .\end{aligned} \tag{29}$$

If one likes, the above result may now be expressed in terms of the so-called dielectric response function. Adler[11] has discussed this function in some detail within the RPA formalism. Let us define

$$K(\varepsilon - is)_{\vec{q}\vec{q}'} = \delta_{\vec{q},\vec{q}'} + \Pi(\varepsilon - is)_{\vec{q}\vec{q}'}\,v(\vec{q}') \quad , \tag{30}$$

and the dielectric response function $K^{-1}(\varepsilon - is)_{\vec{q}\vec{q}'}$ by the relation

$$\sum_{\vec{q}'} K^{-1}(\varepsilon - is)_{\vec{q}\vec{q}_1}\,K(\varepsilon - is)_{\vec{q}_1\vec{q}'} = \delta_{\vec{q},\vec{q}'} \quad . \tag{31}$$

Then from analytic continuation of (10), we obtain

$$\Pi'(\varepsilon - is)_{\vec{q}\vec{q}'}\,v(\vec{q}') = \delta_{\vec{q},\vec{q}'} - K^{-1}(\varepsilon - is)_{\vec{q}\vec{q}'} \quad . \tag{32}$$

Making use of this result in Eq. (29), we find

$$\Gamma_r(E_r) = \mathrm{Im}\,\frac{1}{V}\sum_{\vec{q}\,\vec{q}\,'}\sum_{s} Z_s\,\rho_{rs}(\vec{q})\,\rho_{sr}(-\vec{q}\,')\,v(\vec{q})$$

$$\cdot\, K^{-1}(E_r - E_s - is)_{\vec{q}\,\vec{q}\,'}\,[f^+(E_s)N'(E_r - E_s) + f^-(E_s)N(E_r - E_s)]\ . \tag{33}$$

This result is most simply written out explicitly in the extended zone scheme; one obtains

$$\Gamma_{\vec{k}}(E_{\vec{k}})$$

$$= \mathrm{Im}\,\frac{1}{V}\sum_{\vec{q}}\sum_{\hat{K}\hat{K}'} Z_{\vec{k}-\vec{q}}\,v(\vec{q}+\hat{K})\,M_{\hat{K}'}(\vec{k},\vec{k}-\vec{q})^*\,M_{\hat{K}}(\vec{k},\vec{k}-\vec{q})$$

$$\cdot\, K^{-1}(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - is)_{\vec{q}+\hat{K},\,\vec{q}+\hat{K}'}$$

$$\cdot\, [f^+(E_{\vec{k}-\vec{q}})N'(E_{\vec{k}} - E_{\vec{k}-\vec{q}}) + f^-(E_{\vec{k}-\vec{q}})N(E_{\vec{k}} - E_{\vec{k}-\vec{q}})]\ . \tag{34}$$

In this expression we have suppressed spin indices, $\hat{K}$ and $\hat{K}'$ are reciprocal lattice vectors. The matrix element M in (34) is given by

$$M_{\hat{K}}(\vec{k},\vec{k}-\vec{q}) = \int_{\substack{\text{unit}\\ \text{cell}}} d^3\vec{r}\, e^{i\hat{K}\cdot\vec{r}}\, u^*_{\vec{k}}(\vec{r})\, u_{\vec{k}-\vec{q}}(\vec{r})\ , \tag{35}$$

where the u's are the usual periodic part of the Bloch functions, normalized to unity in a primitive cell.

At zero temperature, (34) reduces to give

$$\Gamma_{\vec{k}}(E_{\vec{k}}) = \mathrm{Im}\,\frac{1}{V}\sum_{\substack{\vec{q} \\ E_{\vec{k}} > E_{\vec{k}-\vec{q}} > E_f}}\sum_{\hat{K}\hat{K}'} Z_{\vec{k}-\vec{q}}\, v(\vec{q}+\hat{K})\, M_{\hat{K}'}(\vec{k},\vec{k}-\vec{q})^{*}\, M_{\hat{K}}(\vec{k},\vec{k}-\vec{q}) \cdot K^{-1}(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - is)_{\vec{q}+\hat{K},\,\vec{q}+\hat{K}'} \,, \tag{36a}$$

for the case $E_{\vec{k}} > E_f$, and

$$\Gamma_{\vec{k}}(E_{\vec{k}}) = -\,\mathrm{Im}\,\frac{1}{V}\sum_{\substack{\vec{q} \\ E_f > E_{\vec{k}-\vec{q}} > E_{\vec{k}}}}\sum_{\hat{K}\hat{K}'} Z_{\vec{k}-\vec{q}}\, v(\vec{q}+\hat{K})\, M_{\hat{K}'}(\vec{k},\vec{k}-\vec{q})^{*}\, M_{\hat{K}}(\vec{k},\vec{k}-\vec{q}) \cdot K^{-1}(E_{\vec{k}} - E_{\vec{k}-\vec{q}} - is)_{\vec{q}+\hat{K},\,\vec{q}+\hat{K}'} \,, \tag{36b}$$

for the case $E_{\vec{k}} < E_f$. Remark that, aside from the renormalization factor Z and the appearance of quasi-particle energies in place of the unperturbed single-particle energies, relation (36a) is exactly Adler's zero temperature result for the decay rate of a particle introduced above and Fermi surface. The interpretation of (36b) is equally clear, namely it represents the decay rate for a hole created below the Fermi surface.

To conclude, we should like to make several comments concerning the dielectric response function. As Adler has discussed, the off-diagonal elements of the dielectric response function give rise to umklapp-local-field corrections. Originally, on the basis of a one-OPW band approximation for aluminum, and using the RPA dielectric response, Adler estimated that umklapp and umklapp-local-field effects might lead

to a correction of 30% or smaller for the lifetime of low-lying excitations, while these effects might be quite important in the plasma production region. Recently,[12] however, he has retracted these estimates and now allows that these effects probably make a rather small correction in both regions. Thus, except perhaps for certain special cases, it would seem that there is justification for ignoring corrections arising from the off-diagonal elements of the dielectric response function. In this case, we may simply write

$$K^{-1}(\varepsilon - is)_{\vec{q}\,\vec{q}\,'} \simeq \frac{\delta_{\vec{q},\vec{q}\,'}}{K(\vec{q}, \varepsilon - is)} \quad , \tag{37}$$

where

$$K(\vec{q}, \varepsilon - is) = 1 + v(\vec{q})\, \Pi(\varepsilon - is)_{\vec{q}\,\vec{q}} \quad , \tag{38}$$

is the usual longitudinal dielectric constant. Using this approximation, (34) reduces to give

$$\Gamma_{\vec{k}}(E_{\vec{k}}) = \frac{1}{V} \sum_{\vec{q}} \sum_{\hat{K}} Z_{\vec{k}-\vec{q}}\, v(\vec{q} + \hat{K})\, \left| M_{\hat{K}}(\vec{k}, \vec{k}-\vec{q}) \right|^2$$

$$\cdot \, \mathrm{Im} \frac{1}{K(\vec{q} + \hat{K},\, E_{\vec{k}} - E_{\vec{k}-\vec{q}} - is)} \left[f^+(E_{\vec{k}-\vec{q}})\, N'(E_{\vec{k}} - E_{\vec{k}-\vec{q}}) + f^-(E_{\vec{k}-\vec{q}}) N(E_{\vec{k}} - E_{\vec{k}-\vec{q}}) \right] . \tag{39}$$

ACKNOWLEDGMENTS

The author wishes to express thanks to D. O. Smith for his encouragement and support, and to K. J. Harte and C. T. Kirk for helpful discussions.

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APPENDIX A

An Approximate Evaluation of Finite Temperature Corrections for a Simple Case

We wish to give an approximate evaluation of (34) for the case of free interacting electrons. We further restrict ourselves to the RPA dielectric response of the electron gas, and shall simply assume that the quasi-particle spectrum may be approximated by the non-interacting dispersion law. At zero temperature, the result we obtain reduces to that quoted by Quinn.

For the case of free electrons, the result (34) becomes simply

$$\Gamma_{\vec{k}}(\epsilon_{\vec{k}}) = \frac{1}{(2\pi)^3} \int d^3\vec{q}\, [f^+(\epsilon_{\vec{k}-\vec{q}}) + N(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}})]$$

$$\cdot\, v(\vec{q})\, \mathrm{Im} \frac{1}{K(\vec{q}, \epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - is)} \quad . \tag{A.1}$$

Letting $d^3\vec{q} = \dfrac{dS_{\vec{q}}\, d\epsilon_{\vec{k}-\vec{q}}}{|\vec{\nabla}_{\vec{q}}\, \epsilon_{\vec{k}-\vec{q}}|}$, where $dS_{\vec{q}}$ is an element of surface area on the surface $\epsilon_{\vec{k}-\vec{q}}$ = constant, we obtain

$$\Gamma_{\vec{k}}(\epsilon_{\vec{k}}) = -\frac{1}{(2\pi)^3} \int_0^\infty d\epsilon_{\vec{k}-\vec{q}}\, [f^+(\epsilon_{\vec{k}-\vec{q}}) + N(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}})$$

$$\cdot \int_{\epsilon_{\vec{k}-\vec{q}} = \mathrm{const.}} \frac{dS_{\vec{q}}\, v(\vec{q})}{|\vec{\nabla}_{\vec{q}}\, \epsilon_{\vec{k}-\vec{q}}|}\, \frac{\mathrm{Im}\, K(\vec{q}, \epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - is)}{|K(\vec{q}, \epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - is)|^2} \tag{A.2}$$

Now for the case $\epsilon_{\vec{k}} \sim \mu$ of low energy excitations, the statistical factors in (A.2) insure that the energy argument of the dielectric constant is small in the region where the integrand is non-negligible. Then using some properties of the well-known RPA dielectric constant,‡ we have

$$\mathrm{Im}\, K(\vec{q}, \epsilon - is) = -\left(\frac{\pi}{4} \frac{k_f k_s^2}{\epsilon_f}\right) \frac{\epsilon}{q^3} \quad , \tag{A.3}$$

$$|K(\vec{q}, \epsilon - is)|^2 \simeq K(\vec{q}, 0)^2 \simeq \left(1 + \frac{k_s^2}{q^2}\right)^2 \quad , \tag{A.4}$$

for sufficiently small ϵ and q. In the expressions above, k_s is the inverse Thomas-Fermi screening length. Making use of these results in (A.2) we obtain

$$\Gamma_{\vec{k}}(\epsilon_{\vec{k}}) = \frac{e^2 k_f k_s^2}{8\pi\epsilon_f} \int_0^\infty d\epsilon_{\vec{k}-\vec{q}} (\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}}) [f^+(\epsilon_{\vec{k}-\vec{q}}) + N(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}})]$$

$$\cdot \int_{\epsilon_{\vec{k}-\vec{q}} = \mathrm{const.}} \frac{dS_{\vec{q}}}{|\vec{\nabla}_{\vec{q}}\, \epsilon_{\vec{k}-\vec{q}}|} \frac{1}{q^5} \frac{1}{\left(1 + \frac{k_s^2}{q^2}\right)^2} \quad . \tag{A.5}$$

‡ It may readily be seen that we are justified in using the zero temperature dielectric constant in this calculation.

Upon carrying out the surface integral, we find

$$\Gamma_{\vec{k}}(\epsilon_{\vec{k}}) = \left(\frac{e^2 k_f}{16}\right)\left(\frac{k_f}{k_s}\right)\left(\frac{k_f}{k}\right)\frac{1}{\epsilon_f^2}$$

$$\cdot \int_0^\infty d\epsilon_{\vec{k}-\vec{q}}\,(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})\,[f^+(\epsilon_{\vec{k}-\vec{q}}) + N(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})] \tag{A.6}$$

$$\cdot \left[\tan^{-1}\frac{q}{k_s} + \frac{k_s q}{k_s^2+q^2}\right]_{|k-P|}^{k+P} ,$$

where $P = \left(\frac{2m}{\hbar^2}\epsilon_{\vec{k}-\vec{q}}\right)^{\frac{1}{2}}$. The remaining integration over $\epsilon_{\vec{k}-\vec{q}}$ is clearly quite complicated. On the other hand, for $\epsilon_{\vec{k}} \sim \mu$, the principal contribution to the integral comes from the region $\epsilon_{\vec{k}-\vec{q}} \sim \mu$, and for such values, the last factor in (A.6) is slowly varying; hence we approximate (A.6) as

$$\Gamma_{\hbar}(\epsilon_{\vec{k}}) \simeq \left(\frac{e^2 k_f}{16}\right)\left(\frac{k_f}{k_s}\right)\left(\frac{k_f}{k}\right)\frac{1}{\epsilon_f^2}\left[\tan^{-1}\frac{2k_f}{k_s} + \frac{2k_f k_s}{k_s^2+4k_f^2}\right] I(\epsilon_{\vec{k}}) , \tag{A.7}$$

with

$$I(\epsilon_{\vec{k}}) = \int_0^\infty d\epsilon_{\vec{k}-\vec{q}}\,(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})\,[f^+(\epsilon_{\vec{k}-\vec{q}}) + N(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})] . \tag{A.8}$$

Then $I(\epsilon_{\vec{k}})$ evaluates to give

$$I(\epsilon_{\vec{k}}) = \frac{1}{2}\,[(\epsilon_{\vec{k}}-\mu)^2 + \pi^2(k_B T)^2 + \ldots] , \tag{A.9}$$

where the terms which have been neglected vanish exponentially as $T \to 0$.

Our final result for $\epsilon_k \sim \mu$ then becomes

$$\Gamma_{\vec{k}}(\epsilon_{\vec{k}}) = \frac{1}{32}\left(e^2 k_f\right)\left(\frac{k_f}{k_s}\right)\left[\tan^{-1}\frac{2k_f}{k_s} + \frac{2k_f k_s}{k_s^2 + 4k_f^2}\right]$$

$$\cdot\left(\frac{k_f}{k}\right)\frac{1}{\epsilon_f^2}\left[(\epsilon_{\vec{k}} - \mu)^2 + \pi^2 (k_B T)^2\right] \quad . \tag{A.10}$$

In a similar manner, by inserting a factor of $\frac{2}{\hbar}(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}})$ into the integrand of (A. 1), we may obtain an approximate expression for the rate of energy loss[13] for an incident particle. The calculation proceeds in complete analogy to the one above; we find

$$\frac{d\epsilon_{\vec{k}}}{dt} = \frac{1}{48}\left(e^2 k_f^2 v_f\right)\left(\frac{k_f}{k_s}\right)\left[\tan^{-1}\frac{2k_f}{k_s} + \frac{2k_f k_s}{k_s^2 + 4k_f^2}\right]$$

$$\cdot\left(\frac{k_f}{k}\right)\frac{1}{\epsilon_f^3}\left[(\epsilon_{\vec{k}} - \mu)^3 + \pi^2 (k_B T)^2 (\epsilon_{\vec{k}} - \mu)\right] \quad , \tag{A.11}$$

so that again, the lowest order finite temperature corrections are of order T^2.

APPENDIX B

Spectral Density Functions and Sum Rules

Making use of relations (4) through (8), and the definitions (11) and (12), it is straightforward to obtain the spectral density functions for the exact one-electron, and polarization propagators; they are, respectively

$$A(E)_{rr'}$$

$$= [e^{\beta(E-\mu)} + 1]\sum_{nm} e^{-\beta(E_n-\mu N_n-\Omega)} \langle n|a^{\dagger}_{r'}|m\rangle\langle m|a_r|n\rangle \delta[E-(E_n-E_m)] \quad , \tag{B.1}$$

$$B(E)_{\vec{q}\vec{q}'}$$

$$= [e^{\beta E} - 1]\frac{1}{V}\sum_{nm} e^{-\beta(E_n-\mu N_n-\Omega)} \langle n|\rho_{\vec{q}'}|m\rangle\langle m|\rho_{-\vec{q}}|n\rangle \delta[E-(E_n-E_m)] \quad . \tag{B.2}$$

It may readily be verified that $B(E)_{\vec{q}\vec{q}'}$ satisfies the following two sum rules

$$\int_{-\infty}^{\infty} dE\, B(E)_{\vec{q}\vec{q}'} = \frac{1}{V}\,\mathrm{Tr}\,\{e^{-\beta(H-\mu N-\Omega)}[\rho_{-\vec{q}}, \rho_{\vec{q}'}]\} = 0 \quad , \tag{B.3}$$

$$\begin{aligned}\int_{-\infty}^{\infty} dE\, E\, B(E)_{\vec{q}\vec{q}'} &= -\frac{1}{V}\,\mathrm{Tr}\left\{e^{-\beta(H-\mu N-\Omega)}\left[\rho_{-\vec{q}},[\rho_{\vec{q}'}, H]\right]\right\} \\ &= \frac{\hbar^2}{m}(\vec{q}\cdot\vec{q}')\frac{1}{V}\,\mathrm{Tr}\,\{e^{-\beta(H-\mu N-\Omega)}\rho_{\vec{q}'-\vec{q}}\} \quad .\end{aligned} \tag{B.4}$$

We note that the right-hand side of (B.4) vanishes unless $\vec{q}$ and $\vec{q}'$ differ

by a reciprocal lattice vector, and for the case $\hat{K} = 0$, we obtain the well-known f-sum rule

$$\int_{-\infty}^{\infty} dE\, E\, B(E)_{\vec{q}\vec{q}} = \frac{\hbar^2 q^2 \bar{n}}{m} \quad . \tag{B.5}$$

Together (B.3) and (B.5) imply the familiar result

$$v(\vec{q})\Pi'(\xi)_{\vec{q}\vec{q}} \to \frac{-\hbar^2\omega_P^2}{\xi^2} \quad \text{as } |\xi| \to \infty \quad .$$

In a similar manner, one verifies the following sum rules for $A(E)_{rr'}$

$$\int_{-\infty}^{\infty} dE\, A(E)_{rr'} = \delta_{rr'} \quad , \tag{B.6}$$

$$\int_{-\infty}^{\infty} dE\, E\, A(E)_{rr'} = \mathrm{Tr}\left\{e^{-\beta(H-\mu N-\Omega)}\left[a_r, [H, a^\dagger_{r'}]\right]_+\right\} \quad . \tag{B.7}$$

If the basis $|r)$ is that which diagonalizes H_o, this last relation becomes

$$\int_{-\infty}^{\infty} dE\, E\, A(E)_{rr'} = \epsilon_r \delta_{rr'}$$

$$+ \sum_{ss'} [(rs|v|r's') - (rs|v|s'r')]\, \mathrm{Tr}\{e^{-\beta(H-\mu N-\Omega)} a^\dagger_s a_{s'}\}$$

$$= \epsilon_r \delta_{rr'} + \sum_{ss'} [(rs|v|r's') - (rs|v|s'r')] \cdot \frac{1}{\beta} \sum_{\ell'} S'_{s's}(z_{\ell'}) e^{z_{\ell'} 0_+}$$

$$= \epsilon_r \delta_{rr'} + G^{(1)}_{rr'} \quad , \tag{B.8}$$

by virtue of Eq. (16). Combining (B.6) and (B.8), we have for $|z| \to \infty$

$$S'_{rr'}(z) \simeq \frac{1}{z} \delta_{rr'} + \frac{1}{z^2} [\epsilon_r \delta_{rr'} + G^{(1)}_{rr'}] \quad . \tag{B.9}$$

Then because

$$G_{rr'}(z) = (z - \epsilon_r)\delta_{rr'} - [S'(z)^{-1}]_{rr'} \quad , \tag{B.10}$$

it is easy to see that

$$G_{rr'}(z) \to G^{(1)}_{rr'} \text{ as } |z| \to \infty \quad .$$

DOCUMENT CONTROL DATA – R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)* Lincoln Laboratory, M. I. T.	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b. GROUP None

3. REPORT TITLE

Finite Temperature Theory for the Attenuation of Quasi-Particle Excitations in Real Metals

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

Technical Note

5. AUTHOR(S) *(Last name, first name, initial)*

Davies, Richard W.

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
14 August 1967	26	13

8a. CONTRACT OR GRANT NO. AF 19(628)-5167 b. PROJECT NO. 649-L c. d.	9a. ORIGINATOR'S REPORT NUMBER(S) Technical Note 1967-39 9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)* ESD-TR-67-336

10. AVAILABILITY/LIMITATION NOTICES

This document has been approved for public release and sale; its distribution is unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
None	Air Force Systems Command, USAF

13. ABSTRACT

The finite temperature generalization of the Quinn, Adler theory for the decay rate of electronic excitations in a normal Fermion system is presented. The theory is developed in terms of quasi-particle parameters and without restriction to a particular approximation, such as RPA, for the dielectric response of the system. The relations derived are pertinent to the lifetime problem in real solids; in particular, local field effects are rigorously taken into account.

14. KEY WORDS

damping   quasi-particle excitations   finite temperature theory